=> FILE REG
FILE 'REGISTRY' ENTERED AT 10:22:37 ON 14 JAN 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 JAN 2004 HIGHEST RN 636984-67-3
DICTIONARY FILE UPDATES: 12 JAN 2004 HIGHEST RN 636984-67-3

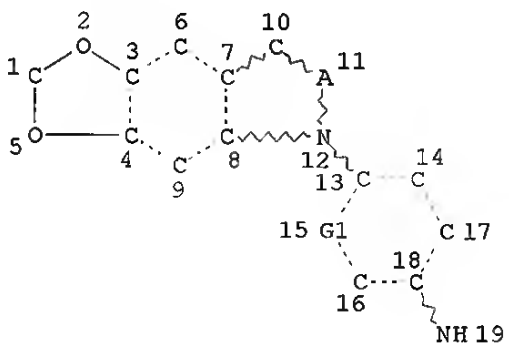
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> D QUE L13
L11 STR



no structures when 2 oxygens are in a ring

VAR G1=N/C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L13 0 SEA FILE=REGISTRY SSS FUL L11

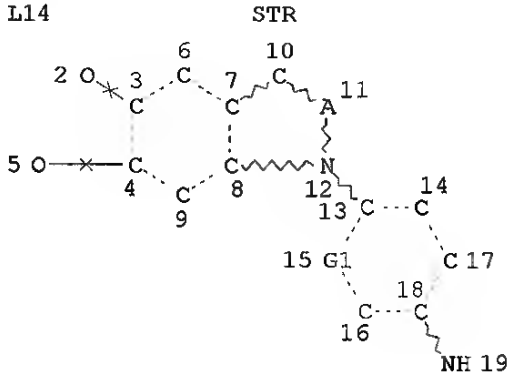
=> FILE HCAPLUS
FILE 'HCAPLUS' ENTERED AT 10:22:54 ON 14 JAN 2004

FILE COVERS 1907 - 14 Jan 2004 VOL 140 ISS 3
FILE LAST UPDATED: 13 Jan 2004 (20040113/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S L16
L17 8 L16

=> D QUE
L14 STR



11 structure/answers when oxygens are ring or chain

VAR G1=N/C
NODE ATTRIBUTES:
NSPEC IS RC AT 2
NSPEC IS RC AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L16 11 SEA FILE=REGISTRY SSS FUL L14
L17 8 SEA FILE=HCAPLUS ABB=ON L16

8 CA references from the 11 structures

=> => D L17 ALL 1-8 HITSTR

L17 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:516257 HCAPLUS

DN 137:95161
ED Entered STN: 11 Jul 2002
TI Indole/indoline hybrid dyes and their application to hair
IN Naumann, Frank; Hollenberg, Detlef; Hoeffkes, Horst; Rose, David
PA Henkel Kgaa, Germany
SO Ger. Offen., 22 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM C09B007-00
ICS C09B069-00; A61K007-13; A61K007-021
CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 27, 62
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10100938	A1	20020711	DE 2001-10100938	20010110
	WO 2002055609	A2	20020718	WO 2002-EP13	20020103
	WO 2002055609	A3	20021227		
	W: AU, BR, CA, CN, CZ, HU, JP, NO, PL, RU, SK, US, VN				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	EP 1349535	A2	20031008	EP 2002-716059	20020103
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
PRAI	DE 2001-10100938	A	20010110		
	WO 2002-EP13	W	20020103		

OS MARPAT 137:95161
AB Indole and indoline hybrid dyes and their precursors of the structure XZY (X = a group derived from a derivative of indole or indoline as melanin precursor; Y = a group from an oxidative dye coupler or developer or a derivative of indole or indoline as melanin precursor; Z = direct bond or spacer group) are suitable for the dyeing of keratinic fibers, in particular human hair. In an example, 4-(5,6-dimethoxy-1-indolinyl)aniline hydrochloride was prepared from 4-nitrofluorobenzene and 5,6-dimethoxyindoline, with formation and reduction of the intermediate 5,6-dimethoxy-1-(4-nitrophenyl)indolline.
ST indole indoline hair dye prodn
IT Alcohols, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(C16-18, Stenol 16/18; surfactant; indole/indoline oxidative hair dyes containing)
IT Alcohols, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(C16-18, ethoxylated, Ceteareth 20; surfactant; indole/indoline oxidative hair dyes containing)
IT Surfactants
(amphoteric; indole/indoline oxidative hair dyes containing)
IT Surfactants
(anionic; indole/indoline oxidative hair dyes containing)
IT Surfactants
(cationic; indole/indoline oxidative hair dyes containing)
IT Hair preparations
(dyes, direct-acting; production of indole/indoline hybrid dyes and their application to hair)
IT Hair preparations
(dyes, oxidative; production of indole/indoline hybrid dyes and their

application to hair)

IT Surfactants
(nonionic; indole/indoline oxidative hair dyes containing)

IT Surfactants
(zwitterionic; indole/indoline oxidative hair dyes containing)

IT 90-15-3, 1-Naphthol 108-46-3, Resorcinol, uses 541-69-5, m-Phenylenediamine dihydrochloride 591-27-5, 3-Aminophenol 66422-95-5, 2-(2,4-Diaminophenoxy)ethanol dihydrochloride 74918-21-1, 1,3-Bis(2,4-diaminophenoxy)propane tetrahydrochloride
RL: TEM (Technical or engineered material use); USES (Uses)
(coupler; indole/indoline oxidative hair dyes containing)

IT **441349-87-7P 441349-88-8P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(dye; production of indole/indoline hybrid dyes and their application to hair)

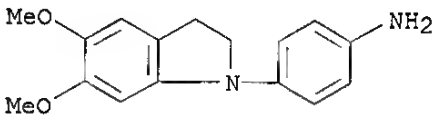
IT 441349-89-9P 441349-90-2P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; production of indole/indoline hybrid dyes and their application to hair)

IT 350-46-9, 4-Nitrofluorobenzene 4548-45-2, 2-Chloro-5-nitropyridine 15937-07-2, 5,6-Dimethoxyindoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; production of indole/indoline hybrid dyes and their application to hair)

IT 9004-82-4, Texapon N28 83138-08-3, Dehyton K
RL: TEM (Technical or engineered material use); USES (Uses)
(surfactant; indole/indoline oxidative hair dyes containing)

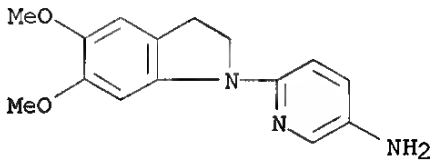
IT **441349-87-7P 441349-88-8P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(dye; production of indole/indoline hybrid dyes and their application to hair)

RN 441349-87-7 HCAPLUS
CN Benzenamine, 4-(2,3-dihydro-5,6-dimethoxy-1H-indol-1-yl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 441349-88-8 HCAPLUS
CN 3-Pyridinamine, 6-(2,3-dihydro-5,6-dimethoxy-1H-indol-1-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

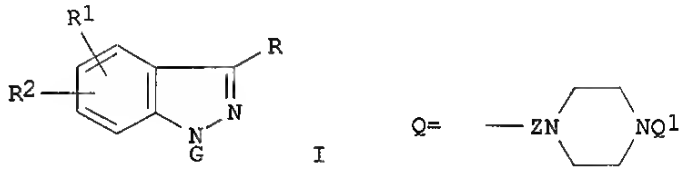


● HCl

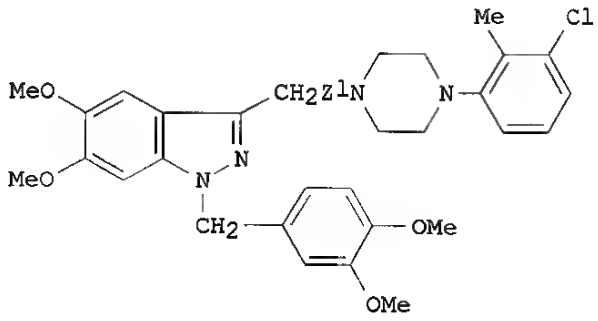
L17 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:694212 HCAPLUS
DN 125:328730
ED Entered STN: 25 Nov 1996
TI Preparation of 3-(piperazinoalkyl)indole derivatives as calmodulin antagonists
IN Hasegawa, Atsushi; Makino, Tooru; Yamamoto, Kenjiro
PA Daiichi Seiyaku Co, Japan
SO Jpn. Kokai Tokkyo Koho, 49 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C07D231-56
ICS C07D401-06; C07D401-12; C07D401-14; C07D403-06; C07D403-12; C07D405-06; C07D405-12; C07D405-14; C07D417-06; C07D491-048; C07D491-056
ICA A61K031-415; A61K031-495; A61K031-505
ICI C07D401-06, C07D213-16, C07D231-56; C07D401-12, C07D213-16
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 08225535	A2	19960903	JP 1995-294071	19951113
PRAI	JP 1994-280963		19941115		

OS MARPAT 125:328730
GI



I



II

AB The title compds. [I; R = Q; wherein Z = single bond, C1-3 alkylene, C2-4 alkenylene, C1-3 hydroxyalkylene, CO, COCO, C1-2 alkylene containing one CO group at the end or middle of the C chain; Q1 = C1-8 alkyl, C3-8 cycloalkyl, (un)substituted aryl, heterocyclyl, diarylmethyl, or aryl-C1-6 alkyl; R1, R2 = C1-6 alkyl or alkoxy, CF3, CF3CH2, CF3O, CF3CH2O, C1-6 alkylthio, alkylsulfinyl, or alkylsulfonyl, C1-6 alkylcarbonyl, C2-7 alkanoylamino, NH2, mono- di(C1-6 alkyl)amino, OH, halo, C2-6 perfluoroalkyl, cyano, NO2, CO2H, C1-6 alkoxycarbonyl, tetrazolyl, SO2NH2, methylenedioxy, ethylenedioxy, morpholinosulfonyl, piperazinosulfonyl, 4-(C1-6 alkyl)piperazinosulfonyl, 4-[mono- or di(C1-6 alkyl)amino]piperidino, 4-aminopiperidino; G = C1-6 alkyl, (un)substituted Ph, PhCO, PhCOCH2, α-hydroxybenzyl, phenyl-C1-6 alkyl, 5-membered aromatic heterocyclyl or heterocyclyl-C1-6 alkyl containing heteroatoms (a) N, O,

or S or (b) one or two N and another N, O, or S, 6-membered aromatic heterocyclyl, heterocyclylcarbonyl, or heterocyclyl-C1-3 alkyl containing one or two N, phenylhydroxyalkyl, or 2-phenylethynyl, tetrazolyl, morpholino, etc.] are prepared These compds. possess calmodulin-inhibitory, antihypoxic, or brain edema-improving activity, inhibit delayed neuronal death in hippocampus, and are useful for the treatment of circulatory diseases or brain diseases. Thus, 5,6-dimethoxy-1-(3,4-dimethoxybenzyl)-1H-indazole-3-acetic acid was condensed with 1-(3-chloro-2-methylphenyl)piperazine using di(2-pyridyl) disulfide and Ph3P in CH2Cl2 at room temperature to give an intermediate (II; Z1 = CO), which was reduced by borane-THF complex in THF under reflux to give the title compound II (Z1 = CH2). The latter compound in vitro showed IC50 of 3.1 μg/mL against Ca/calmodulin-dependent phosphodiesterase.

ST piperazinoalkylindole prepn calmodulin antagonist; hypoxia treatment piperazinoalkylindole; circulatory disease treatment piperazinoalkylindole; brain disease treatment piperazinoalkylindole

IT Brain, disease
Hypoxia
(preparation of 3-(piperazinoalkyl)indole derivs. as calmodulin antagonists for disease treatment)

IT Calmodulins
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of 3-(piperazinoalkyl)indole derivs. as calmodulin antagonists for disease treatment)

IT Circulation
(disorder, preparation of 3-(piperazinoalkyl)indole derivs. as calmodulin antagonists for disease treatment)

IT 160521-92-6P 160521-93-7P 160522-00-9P 162495-46-7P 162495-48-9P
162495-50-3P 162495-91-2P 162495-92-3P 162495-98-9P 162495-99-0P
162496-04-0P 162496-06-2P 162496-07-3P 162496-23-3P 162496-41-5P
162496-42-6P 162496-43-7P 162496-44-8P 162496-45-9P 183314-91-2P
183314-92-3P 183314-93-4P 183314-94-5P 183314-95-6P 183314-96-7P
183314-97-8P 183314-98-9P 183314-99-0P 183315-00-6P 183315-01-7P
183315-02-8P 183315-03-9P 183315-04-0P 183315-05-1P 183315-06-2P
183315-07-3P 183315-08-4P 183315-09-5P 183315-10-8P 183315-11-9P
183315-12-0P 183315-13-1P 183315-14-2P 183315-15-3P 183315-16-4P
183315-17-5P 183315-18-6P 183315-19-7P 183315-20-0P 183315-21-1P
183315-22-2P 183315-23-3P 183315-24-4P 183315-25-5P 183315-26-6P
183315-27-7P 183315-28-8P 183315-29-9P 183315-30-2P 183315-31-3P
183315-32-4P 183315-33-5P 183315-34-6P 183315-35-7P 183315-36-8P
183315-38-0P 183315-41-5P 183315-45-9P 183315-47-1P 183315-48-2P
183315-49-3P 183315-50-6P 183315-51-7P 183315-52-8P 183315-53-9P
183315-54-0P 183315-55-1P 183315-56-2P 183315-57-3P 183315-58-4P
183315-59-5P 183315-60-8P 183315-61-9P 183315-62-0P 183315-63-1P
183315-64-2P 183315-65-3P 183315-66-4P 183315-67-5P 183315-68-6P
183315-69-7P 183315-70-0P 183315-71-1P 183315-72-2P 183315-73-3P
183315-74-4P 183315-75-5P 183315-76-6P 183315-77-7P
183315-78-8P 183315-79-9P 183315-80-2P 183315-81-3P 183315-82-4P
183315-83-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3-(piperazinoalkyl)indole derivs. as calmodulin antagonists for disease treatment)

IT 93-03-8, 3,4-Dimethoxybenzyl alcohol 107-14-2, Chloroacetonitrile 108-59-8, Dimethyl malonate 124-63-0, Mesyl chloride 151-50-8, Potassium cyanide 1822-51-1, 4-Chloromethylpyridine hydrochloride 6315-89-5, 3,4-Dimethoxyaniline 14794-31-1, Ethyl succinyl chloride 29281-06-9 35386-24-4, N-(2-Methoxyphenyl)piperazine 54711-70-5, 1-(3-Chloro-2-methylphenyl)piperazine 98224-26-1, 1-(7-Benzofuranyl)piperazine 103057-10-9, 4-Chloromethyl-1-tritylimidazole 183315-95-9, Methyl 5,6-dimethoxyindazole-3-acetate 183315-96-0 183315-98-2, 4-Morpholinosulfonamidobenzyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 3-(piperazinoalkyl)indole derivs. as calmodulin antagonists for disease treatment)

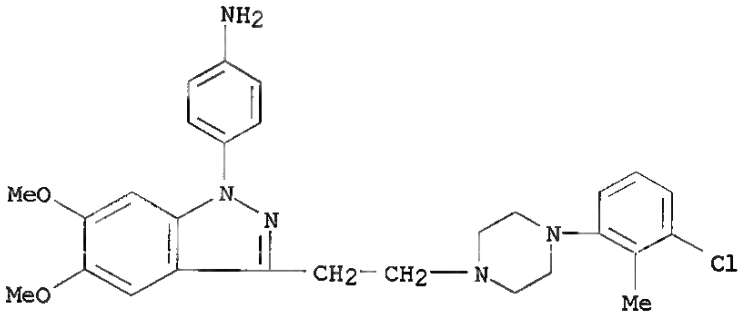
IT 7306-46-9P, 3,4-Dimethoxybenzyl chloride 68438-33-5P 98205-73-3P
160521-88-0P 160521-89-1P 160521-90-4P 160521-91-5P 160521-95-9P
160521-99-3P 162496-66-4P 183315-84-6P 183315-85-7P 183315-86-8P
183315-87-9P 183315-88-0P 183315-89-1P 183315-90-4P 183315-91-5P
183315-92-6P 183315-93-7P 183315-94-8P 183315-97-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-(piperazinoalkyl)indole derivs. as calmodulin antagonists for disease treatment)

IT **183315-74-4P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3-(piperazinoalkyl)indole derivs. as calmodulin antagonists for disease treatment)

RN 183315-74-4 HCAPLUS

CN Benzenamine, 4-[3-[2-[4-(3-chloro-2-methylphenyl)-1-piperazinyl]ethyl]-5,6-dimethoxy-1H-indazol-1-yl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L17 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1991:448658 HCAPLUS

DN 115:48658

ED Entered STN: 10 Aug 1991

TI Comparative study of the behavior of 1H-indazoles and 1-(p-aminophenyl)indazoles under electron impact

AU Erra-Balsells, R.

CS Fac. Cienc. Exactas Nat., Univ. Buenos Aires, Buenos Aires, 1430, Argent.

SO Organic Mass Spectrometry (1991), 26(4), 293-7
CODEN: ORMSBG; ISSN: 0030-493X

DT Journal

LA English

CC 22-8 (Physical Organic Chemistry)

AB The electron impact mass spectrometric fragmentation pathways for several 1H-indazoles and 1-(p-aminophenyl)indazoles were investigated. An interesting relationship between the substitution pattern in the framework of the indazole derivs. and the fragmentation patterns was observed

ST mass spectra indazole; aminophenylindazole mass spectra

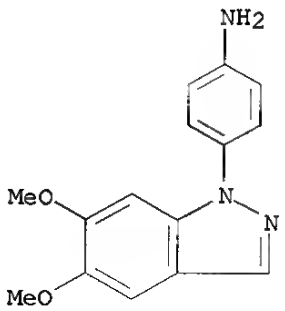
IT Mass spectra
(of indazoles and of (aminophenyl)indazoles)

IT Substituent effect
(on mass spectra of indazoles)

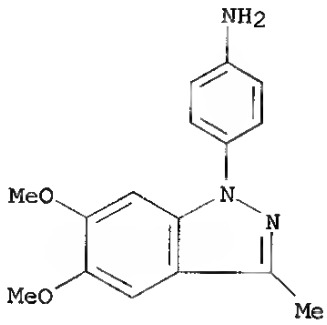
IT 3176-62-3 7746-23-8 7746-24-9 **7746-25-0** **7746-26-1**
7746-27-2 7746-28-3 7746-29-4 7746-30-7 7746-31-8 7788-03-6
7788-04-7 16640-81-6 16640-83-8 16640-87-2 16640-89-4 16640-90-7
16640-93-0 16641-04-6 16641-06-8 33101-36-9 110967-33-4
RL: PRP (Properties)
(mass spectrum of)

IT **7746-25-0** **7746-26-1**

RL: PRP (Properties)
(mass spectrum of)
RN 7746-25-0 HCAPLUS
CN Benzenamine, 4-(5,6-dimethoxy-1H-indazol-1-yl)- (9CI) (CA INDEX NAME)



RN 7746-26-1 HCAPLUS
CN Benzenamine, 4-(5,6-dimethoxy-3-methyl-1H-indazol-1-yl)- (9CI) (CA INDEX NAME)



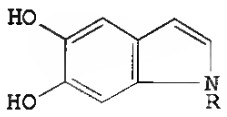
L17 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:204467 HCAPLUS
DN 112:204467
ED Entered STN: 26 May 1990
TI The use of N-substituted-5,6-dihydroxyindoles as a hair coloring agent
IN Schultz, Thomas M.; Brown, Keith C.; Murphy, Bryan P.; Mayer, Alice A.; Lim, Mu Ill
PA Bristol-Myers Co., USA
SO Eur. Pat. Appl., 8 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM A61K007-13
CC 62-3 (Essential Oils and Cosmetics)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 335477	A2	19891004	EP 1989-300514	19890119
	EP 335477	A3	19900418		

	EP 335477	B1	19930721		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	CA 1324320	A1	19931116	CA 1988-572311	19880718
	AT 91621	E	19930815	AT 1989-300514	19890119
	ES 2058487	T3	19941101	ES 1989-300514	19890119
	JP 01254617	A2	19891011	JP 1989-24141	19890203
	JP 2855205	B2	19990210		
PRAI	US 1988-175565		19880331		
	EP 1989-300514		19890119		

OS MARPAT 112:204467

GI



I

AB A method for dyeing hair comprises contacting the hair with a solution of a H2O-soluble metal ion followed by contacting the hair with an N-substituted 5,6-dihydroxyindole I [R = C1-8 alkyl, hydroxy- or aminoalkyl, (substituted) amino- or nitroaryl], or the reverse. Hair is colored light golden to light reddish brown to dark auburn to black, depending on the nature of the metal ion and its concentration, and the pH of the dye. Blended gray hair was treated with pH 9, 1.0% CuSO4 for 5 min at room temperature, and then with a pH 3 1.0% solution of N-methyl-5,6-dihydroxyindole (II) for 5 min, resulting in a dark charcoal grey color. The same type hair treated the same as above but with II at pH 12 resulted in a black color.

ST hydroxyindole metal ion hair dye; methyldihydroxyindole copper ion hair dye; indole methyldihydroxy copper ion hair dye

IT Metals, biological studies
RL: BIOL (Biological study)
(dihydroxyindole derivs. in combination with, as hair dyes)

IT Hair preparations
(dyes, dihydroxyindole derivs. in combination with metal ions as)

IT 7758-98-7, Cupric sulfate, biological studies
RL: BIOL (Biological study)
(N-methyl-dihydroxyindole in combination with, as hair dye)

IT 3131-52-0D, 5,6-Dihydroxyindole, N-substituted 4821-00-5, N-Methyl-5,6-dihydroxyindole 99855-01-3, N-Isopropyl-5,6-dihydroxyindole 126972-29-0, N-(2,4-Dinitrophenyl)-5,6-dihydroxyindole 126972-30-3, N-(4-Nitrophenyl)-5,6-dihydroxyindole **126972-31-4**, N-(4-Aminophenyl)-5,6-dihydroxyindole
RL: BIOL (Biological study)
(as hair dye in combination with metal ions)

IT 7439-89-6D, Iron, mixture with dihydroxyindole derivs., biological studies 7439-92-1D, Lead, mixture with dihydroxyindole derivs., biological studies 7439-96-5D, Manganese, mixture with dihydroxyindole derivs., biological studies 7440-02-0D, Nickel, mixture with dihydroxyindole derivs., biological studies 7440-05-3D, Palladium, mixture with dihydroxyindole derivs., biological studies 7440-22-4D, Silver, mixture with dihydroxyindole derivs., biological studies 7440-31-5D, Tin, mixture with dihydroxyindole derivs., biological studies 7440-32-6D, Titanium, mixture with dihydroxyindole derivs., biological studies 7440-47-3D, Chromium, mixture with dihydroxyindole derivs., biological studies 7440-48-4D, Cobalt, mixture with dihydroxyindole derivs., biological studies

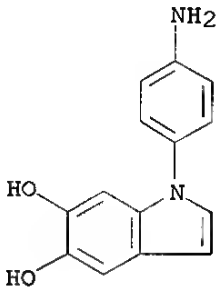
7440-50-8D, Copper, mixture with dihydroxyindole derivs., biological studies
7440-57-5D, Gold, mixture with dihydroxyindole derivs., biological studies
7440-66-6D, Zinc, mixture with dihydroxyindole derivs., biological studies
7440-69-9D, Bismuth, mixture with dihydroxyindole derivs., biological studies
RL: BIOL (Biological study)
(as hair dyes)

IT 557-34-6, Zinc(II) acetate 638-38-0, Manganese(II) acetate 7761-88-8, Silver nitrate, biological studies 10028-22-5, Ferric sulfate
RL: BIOL (Biological study)
(N-methyl-dihydroxyindole in combination with, as hair dye)

IT **126972-31-4**, N-(4-Aminophenyl)-5,6-dihydroxyindole
RL: BIOL (Biological study)
(as hair dye in combination with metal ions)

RN 126972-31-4 HCAPLUS

CN 1H-Indole-5,6-diol, 1-(4-aminophenyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1979:212244 HCAPLUS

DN 90:212244

ED Entered STN: 12 May 1984

TI Polarographic study of some carbazolo- and dibenzofuranoquinones in solutions of varying pH at the DME

AU Etaiw, Safaa Hassan

CS Fac. Sci., Tanta Univ., Tanta, Egypt

SO Annali di Chimica (Rome, Italy) (1978), 68(5-6), 421-31
CODEN: ANCRAI; ISSN: 0003-4592

DT Journal

LA English

CC 72-11 (Electrochemistry)
Section cross-reference(s): 22, 27, 43

AB The polarog. behavior of carbazoloquinone and dibenzofuranquinone derivs. in ethanolic-universal buffer mixts. was studied at the dropping Hg electrode. The polarograms consist of a single reduction wave in solns. having pH values from 3.0 to 9.5, but of 2 daughter waves in strong alkaline media. The electrode reaction involves the up-take of 2 electrons and 2 protons. The effect of mol. structure and pH on El/2, as well as the reduction mechanism, are discussed. Also, correlations between the electrochem. and spectroscopic behavior of these compds. were investigated.

ST polarog carbazolo quinone benzo furan

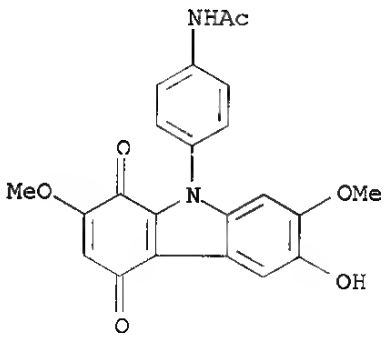
IT Reduction, electrochemical
(of carbazoloquinone and dibenzofuranoquinone derivs.)

IT 36783-65-0 36783-66-1 36783-67-2 36783-68-3 36820-07-2
43042-27-9 43042-29-1 43042-30-4 43042-31-5 50433-97-1
51620-25-8 51620-47-4 51620-56-5 54808-25-2D, derivs.
62983-28-2 64513-58-2 70208-89-8 70377-05-8D, derivs.
RL: PRP (Properties)
(polarog. of, in ethanol media)

IT **62983-28-2**
RL: PRP (Properties)
(polarog. of, in ethanol media)

RN 62983-28-2 HCAPLUS

CN Acetamide, N-[4-(1,4-dihydro-6-hydroxy-2,7-dimethoxy-1,4-dioxo-9H-carbazol-9-yl)phenyl]- (9CI) (CA INDEX NAME)



L17 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1977:421795 HCAPLUS

DN 87:21795

ED Entered STN: 12 May 1984

TI The electronic and vibrational spectra of some N-substituted carbazoloquinones

AU Issa, I. M.; El-Samahy, A. A.; Issa, R. M.; El-Kashef, H. S.; Etaiw, S. H.

CS Fac. Sci., Tanta Univ., Tanta, Egypt

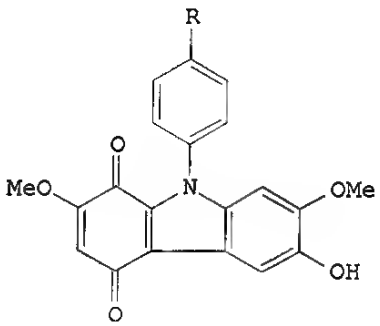
SO Revue Roumaine de Chimie (1977), 22(3), 411-19
CODEN: RRCHAX; ISSN: 0035-3930

DT Journal

LA English

CC 22-2 (Physical Organic Chemistry)

GI



I

AB The bands in the UV of I (R = H, NHAc, OMe, OH, Me, Cl, CO2H) are assigned and the solvent effects discussed. The 480 nm band is assigned to the intramol. charge-transfer from the N atom to the quinone ring, based on solvent and substituent effects. The pK of I, λmax for I and its anion, and the ε for I and its anion are linearly related to σ. The IR of I are discussed.

ST UV carbazoloquinone substituent effect; IR carbazoloquinone substituent effect; acidity carbazoloquinone; charge transfer carbazoloquinone; LFER carbazoloquinone UV IR

IT Carbonyl group
(IR of, in N-substituted carbazoloquinones)

IT Linear free energy relationship
(for UV and IR of N-substituted carbazoloquinones)

IT Reaction constant
(for acidity of hydroxycarbazoloquinones)

IT Ultraviolet and visible spectra
(of N-substituted carbazoloquinones, solvent and substituent effects on)

IT Ionization in liquids
(of N-substituted hydroxycarbazoloquinones, UV in relation to)

IT Solvation
(of carbazoloquinones in ground and excited states, charge-transfer in relation to)

IT Infrared spectra
(of carbazoloquinones, substituent effect on)

IT Free energy
(of ionization of hydroxycarbazoloquinones)

IT Energy level transition
(electronic, of N-substituted carbazoloquinones)

IT Electron exchange
(intramol., in carbazoloquinones, solvent and substituent effects on)

IT Energy level transition
(vibrational, of N-substituted carbazoloquinones)

IT 62983-29-3 62983-30-6 62983-31-7 62983-32-8 62983-33-9
63026-84-6
RL: PRP (Properties)
(UV of)

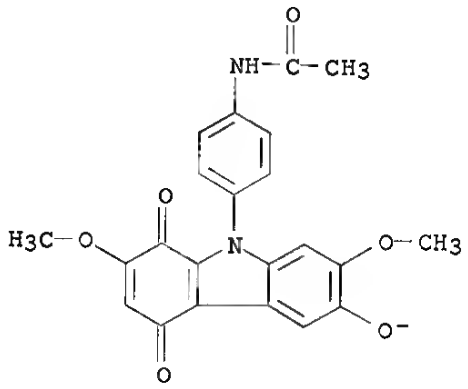
IT 43042-33-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with anilines)

IT 36783-68-3 36820-07-2 51620-25-8 51620-47-4 51620-56-5
62983-28-2
RL: PRP (Properties)
(dissociation constant, IR, and UV of, solvent effect on)

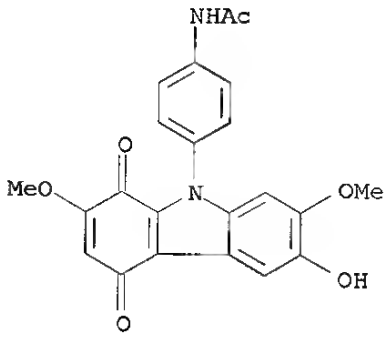
IT **63026-84-6**
RL: PRP (Properties)
(UV of)

RN 63026-84-6 HCAPLUS

CN Acetamide, N-[4-(1,4-dihydro-6-hydroxy-2,7-dimethoxy-1,4-dioxo-9H-carbazol-9-yl)phenyl]-, ion(1-) (9CI) (CA INDEX NAME)



IT 62983-28-2
RL: PRP (Properties)
(dissociation constant, IR, and UV of, solvent effect on)
RN 62983-28-2 HCAPLUS
CN Acetamide, N-[4-(1,4-dihydro-6-hydroxy-2,7-dimethoxy-1,4-dioxo-9H-carbazol-9-yl)phenyl]- (9CI) (CA INDEX NAME)



L17 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:95653 HCAPLUS
DN 80:95653
ED Entered STN: 12 May 1984
TI Heterocyclic quinones. III. New carbazoloquinones from dimethoxydiquinone and various substituted amino compounds
AU Hammam, Ahmed S.
CS Dep. Chem., Univ. Assiut, Assiut, Egypt
SO Egyptian Journal of Chemistry (1972), 15(5), 391-410
CODEN: EGJCA3; ISSN: 0449-2285
DT Journal
LA English
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 22, 1, 34
GI For diagram(s), see printed CA Issue.
AB The reaction of amino compds. containing deactivating groups (e.g., p-O2NC6H4NH2, p-H2NC6H4COMe, amino acids, or acid amides) with 4,4'-dimethoxydiquinone (I) failed. I and amino acids did react in the

presence of Na2CO3, NaHCO3, or pyridine to give acidic carbazoloquinones. I and o-H2NC6H4CO2H gave the blue-violet reduction product II in alc., the carbazoloquinone (III, R = o-HO2CC6H4) in ethylene glycol-pyridine, and the quinone (IV) in ethylene glycol. I and NH2OH gave III (R = OH). I and NH2NH2 gave II. Approx. ten III were prepared including III (R = p-HO3SC6H4) (V) which was a tranquilizer with ED50 250 mg/kg and LD50 825 mg/kg; V was also a potentiator for tranquilizers. The substituent effect on the uv spectra of III was discussed.

ST methoxydiquinone amine condensation; carbazoloquinone tranquilizer; UV carbazoloquinone substituent effect; amino acid methoxydiquinone condensation

IT Tranquilizers
(carbazoloquinones as)

IT Ultraviolet and visible spectra
(of carbazoloquinones, substituent effect on)

IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(with dimethoxydiquinone)

IT 51620-26-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and tranquilizer properties of)

IT 43042-31-5P 51620-27-0P 51620-47-4P 51620-48-5P 51620-49-6P
51620-50-9P 51620-51-0P 51620-52-1P 51620-53-2P 51620-54-3P
51620-55-4P 51620-56-5P 51620-57-6P 51620-58-7P **51620-59-8P**
51620-60-1P 51620-61-2P 51620-62-3P 51620-63-4P
51620-64-5P 51620-65-6P 51620-66-7P 51620-67-8P 51620-68-9P
51620-69-0P 51620-70-3P 51620-71-4P 51620-72-5P 51620-73-6P
51620-74-7P 51620-75-8P 51823-28-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 43042-33-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amines)

IT 74-89-5 75-04-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbazoloquinones)

IT 56-40-6, reactions 90-04-0 95-51-2 106-40-1 106-47-8 106-50-3, reactions 107-95-9 118-92-3 121-57-3 123-30-8 150-13-0 540-37-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethoxydiquinone)

IT 51620-25-8 51620-26-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethylamine)

IT 51620-46-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyleneamine)

IT 302-01-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of dimethoxydiquinone by)

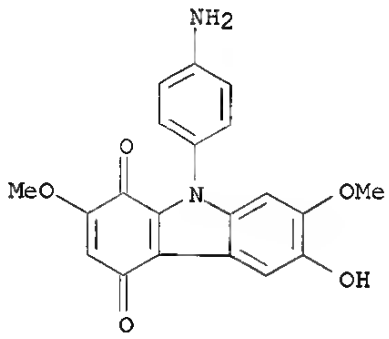
IT 7803-49-8, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(with dimethoxydiquinone)

IT **51620-59-8P 51620-60-1P 51620-61-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

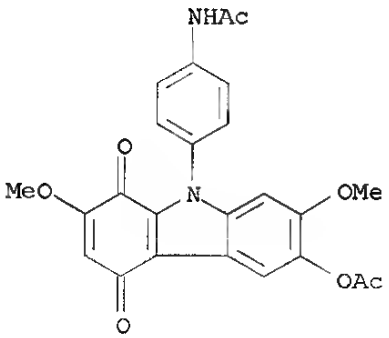
RN 51620-59-8 HCAPLUS

CN 1H-Carbazole-1,4(9H)-dione, 9-(4-aminophenyl)-6-hydroxy-2,7-dimethoxy-

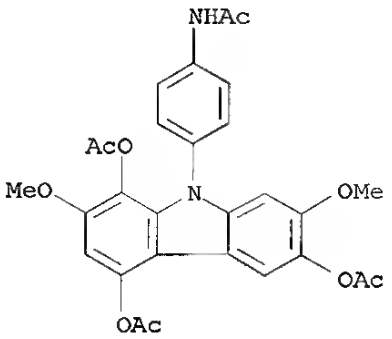
(9CI) (CA INDEX NAME)



RN 51620-60-1 HCAPLUS
CN Acetamide, N-[4-[6-(acetyloxy)-1,4-dihydro-2,7-dimethoxy-1,4-dioxo-9H-carbazol-9-yl]phenyl]- (9CI) (CA INDEX NAME)



RN 51620-61-2 HCAPLUS
CN Acetamide, N-[4-[1,4,6-tris(acetyloxy)-2,7-dimethoxy-9H-carbazol-9-yl]phenyl]- (9CI) (CA INDEX NAME)



L17 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1966:499303 HCAPLUS

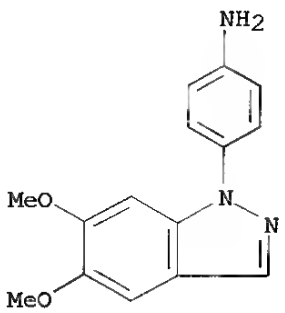
DN 65:99303
OREF 65:18573g-h
ED Entered STN: 22 Apr 2001
TI Synthesis of indazoles using polyphosphoric acid. I
AU Dennler, E. B.; Frasca, A. R.
CS Lab. Quim. Org. Fac. Cienc. Exact. Nat., Buenos Aires
SO Tetrahedron (1966), 22(9), 3131-41
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 65:99303
AB Indazoles were synthesized from nitrophenylhydrazones of several acetophenones, benzaldehydes and benzophenones, employing polyphosphoric acid as catalyst.
IT Catalysts and Catalysis
(in indazole synthesis, polyphosphoric acid as)
IT Acetophenone, 2',5'-dimethoxy-, (p-nitrophenyl)hydrazone
Thiazolo[5,4-f]quinoline-8-carboxylic acid, 7-(o-hydroxyphenyl)-2-methyl-, δ-lactone
IT 271-44-3, Indazole
(derivs., synthesis with polyphosphoric acid catalysts)
IT 7664-38-2, Phosphoric acid
(polyphosphoric acid catalycts, in indazole synthesis)
IT 1575-21-9, 1H-Indazole, 1-(p-nitrophenyl)-3-phenyl- 2675-26-5, Acetophenone, 4'-bromo-, (p-nitrophenyl)hydrazone 2675-27-6, Acetophenone, 4'-ethoxy-, (p-nitrophenyl)hydrazone 3176-62-3, 1H-Indazole, 3-methyl- 4106-21-2, 1H-Indazole, 3-methyl-1-(p-nitrophenyl)- 4106-23-4, 1H-Indazole, 6-methoxy-3-methyl-1-(p-nitrophenyl)- 7714-54-7, Acetophenone, 2',4'-dimethyl-, (m-nitrophenyl)hydrazone 7714-55-8, Acetophenone, (o-nitrophenyl)hydrazone 7714-56-9, Acetophenone, 4'-chloro-, (o-nitrophenyl)hydrazone 7746-02-3, Thiazolo[4,5-f]quinoline-8-carboxylic acid, 7-(o-hydroxyphenyl)-2-methyl-, δ-lactone 7746-04-5, 1(2H)-Naphthalenone, 3,4-dihydro-, 6-benzothiazolylhydrazone 7746-07-8, 1(2H)-Naphthalenone, 3,4-dihydro-6,7-dimethyl-, (2-methyl-6-benzothiazolyl)hydrazone 7746-10-3, 1H-Indazole, 4-chloro-3-methyl-1-(p-nitrophenyl)- 7746-11-4, 1H-Indazole, 6-bromo-3-methyl-1-(p-nitrophenyl)- 7746-12-5, 1H-Indazole, 3,6-dimethyl-1-(p-nitrophenyl)- 7746-13-6, 1H-Indazole, 6-ethyl-3-methyl-1-(p-nitrophenyl)- 7746-15-8, 1H-Indazole, 6-ethoxy-3-methyl-1-(p-nitrophenyl)- 7746-16-9, 1H-Indazole, 3-methyl-1-(p-nitrophenyl)-6-phenyl- 7746-17-0, 1H-Indazole, 3,4,6-trimethyl-1-(p-nitrophenyl)- 7746-18-1, 1H-Indazole, 4,6-dimethoxy-3-methyl-1-(p-nitrophenyl)- 7746-19-2, 1H-Indazole, 5,6-dimethoxy-3-methyl-1-(p-nitrophenyl)- 7746-20-5, 1H-Indazole, 6-methoxy-1-(p-nitrophenyl)- 7746-21-6, 1H-Indazol-6-ol, 5-methoxy-1-(p-nitrophenyl)- 7746-22-7, 1H-Indazole, 5,6-dimethoxy-1-(p-nitrophenyl)- 7746-23-8, 1H-Indazole, 1-(p-aminophenyl)-3,6-dimethyl- 7746-24-9, 1H-Indazole, 1-(p-aminophenyl)-6-methoxy-3-methyl- **7746-25-0**, 1H-Indazole, 1-(p-aminophenyl)-5,6-dimethoxy- **7746-26-1**, 1H-Indazole, 1-(p-aminophenyl)-5,6-dimethoxy-3-methyl- 7746-27-2, 1H-Indazole, 6-bromo-3-methyl- 7746-28-3, 1H-Indazole, 3,6-dimethyl- 7746-29-4, 1H-Indazole, 6-methoxy-3-methyl- 7746-31-8, 1H-Indazole, 5,6-dimethoxy-3-methyl- 7746-32-9, 1H-Indazole, 1,1'-(azoxydi-p-phenylene)bis[3-methyl- 7746-33-0, 1H-Indazole, 1,1'-(azodi-p-phenylene)bis[3-methyl- 7746-35-2, 1H-Indazole, 3-methyl-1-(m-

nitrophenyl)- 7746-37-4, 1H-Indazole, 6-chloro-3-methyl-1-(m-nitrophenyl)- 7746-38-5, Indole, 2-(p-chlorophenyl)-4-nitro- 7746-39-6, Indole, 2-(p-chlorophenyl)-6-nitro- 7746-40-9, 1H-Indazole, 3,6-dimethyl-1-(m-nitrophenyl)- 7746-41-0, Indole, 4-nitro-2-p-tolyl- 7746-42-1, Indole, 6-nitro-2-p-tolyl- 7746-43-2, 1H-Indazole, 6-methoxy-3-methyl-1-(m-nitrophenyl)- 7746-44-3, 1H-Indazole, 3-methyl-1-(m-nitrophenyl)-6-phenyl- 7746-45-4, 1H-Indazole, 3,4,6-trimethyl-1-(m-nitrophenyl)- 7746-47-6, Acetophenone, 3'-hydroxy-, (p-nitrophenyl)hydrazone 7746-48-7, Acetophenone, 4'-hydroxy-, (p-nitrophenyl)hydrazone 7746-49-8, Acetophenone, 4'-ethyl-, (p-nitrophenyl)hydrazone 7746-51-2, Acetophenone, 4'-phenyl-, (p-nitrophenyl)hydrazone 7746-52-3, Acetophenone, 2'-nitro-, (p-nitrophenyl)hydrazone 7746-53-4, Acetophenone, 4'-hydroxy-, (p-nitrophenyl)hydrazone, acetate (ester) 7746-54-5, Acetophenone, 2',4'-dimethyl-, (p-nitrophenyl)hydrazone 7746-55-6, Acetophenone, 2',4'-dimethoxy-, (p-nitrophenyl)hydrazone 7746-57-8, Acetophenone, 2',4',5'-trimethyl-, (p-nitrophenyl)hydrazone 7746-58-9, Acetophenone, (m-nitrophenyl)hydrazone 7746-59-0, Acetophenone, 4'-chloro-, (m-nitrophenyl)hydrazone 7746-60-3, Acetophenone, 4'-methyl-, (m-nitrophenyl)hydrazone 7746-61-4, Acetophenone, 4'-methoxy-, (m-nitrophenyl)hydrazone 7759-57-1, Thiazolo[4,5-f]quinoline-8-carboxylic acid, 7-(o-hydroxyphenyl)-, δ-lactone 7759-58-2, Thiazolo[5,4-f]quinoline-8-carboxylic acid, 7-(o-hydroxyphenyl)-, δ-lactone 7765-63-1, Acetophenone, 4'-phenyl-, (m-nitrophenyl)hydrazone 7767-82-0, Acetophenone, 4'-methyl-, (o-nitrophenyl)hydrazone 7767-83-1, Acetophenone, 4'-methoxy-, (o-nitrophenyl)hydrazone 7788-02-5, 1H-Indazole, 6-methoxy-3-(p-methoxyphenyl)-1-(p-nitrophenyl)- 7788-03-6, 1H-Indazole, 1-(p-aminophenyl)-3-methyl- 7788-04-7, 1H-Indazole, 1-(p-aminophenyl)-6-bromo-3-methyl- 10550-35-3, 1H-Indazole, 6-chloro-3-methyl-1-(p-nitrophenyl)- 10550-36-4, 1H-Indazol-6-ol, 3-methyl-1-(p-nitrophenyl)-, acetate (ester) 14888-76-7, 1H-Indazole, 3-methyl-, picrate 90557-61-2, 1H-Indazole, 6,7-dimethoxy-
(preparation of)

IT **7746-25-0**, 1H-Indazole, 1-(p-aminophenyl)-5,6-dimethoxy-
7746-26-1, 1H-Indazole, 1-(p-aminophenyl)-5,6-dimethoxy-3-methyl-
(preparation of)

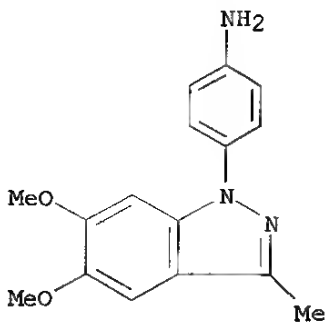
RN 7746-25-0 HCAPLUS

CN Benzenamine, 4-(5,6-dimethoxy-1H-indazol-1-yl)- (9CI) (CA INDEX NAME)



RN 7746-26-1 HCAPLUS

CN Benzenamine, 4-(5,6-dimethoxy-3-methyl-1H-indazol-1-yl)- (9CI) (CA INDEX NAME)


NH2
MeO
MeO
N
N
Me

=>